

1,1,2,2-Tetrahydroperfluoro-1-decanol
678-39-7 | DTXSID7029904

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 61.8 °C

Global applicability domain: Outside

Local applicability domain index: 3.48e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Nonanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9- hexadecafluoro- Measured: 56.0 Predicted: 54.2</div>	<div>Image not found</div> <div>PFOA Measured: 55.0 Predicted: 53.2</div>	<div>Image not found</div> <div>Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7- dodecafluoro- Measured: 34.0 Predicted: 32.9</div>
<div>Image not found</div> <div>Perfluorododecanoic acid Measured: 108 Predicted: 103</div>	<div>Image not found</div> <div>Sulfluramid Measured: 96.0 Predicted: 92.5</div>	